ANALYTICAL STUDY OF THE BAND GAP AND OPTICAL CHARACTERISTICS OF COPPER SULPHIDE THIN FILM: EXPERIMENT AND COMPUTATION

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Received 01 June 2015; accepted 20 July 2015

Abstract
In this work, the analytical study of optical properties and band gap of copper sulphide thin film were carried out comparatively using two different but related depositional techniques done at room temperature. The techniques were (a) successive ionic layer adsorption and reaction and (b) chemical bath deposition. The film was characterized with emphasis on the optical properties within the spectral range of ultraviolet -infrared region of electromagnetic spectrum. Absorption coefficient depicts a maximal value of the band gap ranging from 1.45eV to 3.33 eV. Theoretically, scalar wave equation was used to analyze the behavior of wave propagated through the copper sulphide thin film for which computation of the optical properties such spectral transmittance, reflectance were computed. The band gap of the thin film was also computed for which all the computation was carried out within the same spectral range. In the analysis, it was observed that there was no significant deviation between the band gap obtained from the two different depositional techniques and the computed band gap.

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Key words: Analytical study, copper Sulphide, optical properties, band gap, Scalar wave, deposition, computation, wave propagation.

INTRODUCTION
Copper sulphide belongs to II-IV compound semiconductor material which forms five stable phases such as corellite (CuS), anilite (Cu$_{1.7}$S), digenite (Cu$_{1.8}$S), djurteite (Cu$_{1.95}$S) and chalcocite (Cu$_2$S) at room temperature with different crystal structure such as hexagonal, orthorhombic, pseudocubic and tetragonal depending on x if it is defined in the form Cu$_x$S, (Pathan and Lokhande, 2004).

Copper sulphide thin film has received tremendous attention due to the discovery of its application as photothermal conversion, electroconductive electrode, microwave shielding and solar control coating [Grozdanov and Najdosi, 1995; Suarez and Nair, 1996; Nascus et al., 1997). Its usefulness as photo-detector and in photovoltaic applications cannot be overemphasized. As a result, many material scientists had worked on copper sulphide thin film using different approaches. For instance, deposition of Cu$_x$S thin film using successive ionic layer adsorption and reaction (SILAR) method [Lindros et al, 2000; Sartale and Lokhande, 2000a; Pathan and Lokhande, 2001a] and chemical bath deposition (CBD) [Ugwu, 2009].

Apart from different experimental technique already used, in characterization and study of copper sulphide thin film, theoretical analysis and assessment had also been used in the study of copper sulphide [Ugwu, 2014]. To carry out the analysis, the behavior of propagated electromagnetic wave through thin film medium with non-homogenous and homogenous characteristics were studied using Lippmann-Schwinger and its counterpart Dyson’s equations in which a method of propagating an input field over a small distance representing the thickness of thin film medium was invoked in conjunction the variation of refractive index and dielectric constant. Close look on this concept affirms the true fact of the influence of the solid state properties on the electromagnetic wave behaviour as it propagates through the film [Dograia et al. 2001; Kim et al, 1990; Valanju et al, 2007; Pendery and Smith, 2003].

Munce (2006) has also not only use CBD to develop copper sulphide, but has also analyzed the growth kinetic during which he critically invested the growth mechanism using in-situ crystal microbalance (QCM) by considering the initial values of growth rate as a function of the main reaction parameters such as temperature,
concentration of the reactants [Paravee and Chih-hung, 2013].

In this study, we intend to analytically study the optical and solid state properties of CuS using a scalar wave equation to obtain a theoretical express that would enhance the computation of the parameters to be used in obtaining the optical and solid state properties the thin film which would be compared to experimentally developed thin film deposited using SILAR and CBD.

**Material and Method**

Copper sulphide thin film was developed using successive, ionic layer adsorption and reaction and chemical bath deposition on a glass substrate at a room temperature using thiourea, sodium acetates, triethanolamine, copper sulphate and de-ionized water at given concentration respectively.

After the deposition, the characterization of the thin film was carried out with the following properties in mind, surface morphology, composition and structure using scanning electron microscope coupled with x-ray diffraction analysis while the optical transmission and optical band gap of the thin film were done using UV-VS absorption measurement.

In the case of the theoretical analysis, general wave equation

\[ \nabla^2 \psi(x) - \frac{k^2}{\varepsilon} \psi(x) = 0 \]

In one-dimension was used to derive the governing equation of the model

\[ \nabla^2 \psi(x) + \sigma \varepsilon \mu \Delta \varepsilon \psi(x) = 0 \]

Whose solution is given as

\[ \psi(x) = \int G(x,x') V(x') \psi(x') dx' \]

Which is an integral equation describing the behaviour of the wave propagating through the thin film. Complete integration of this equation depict the value, \( \psi(x) \) of the wave whose behaviour is characterized by the dielectric perturbation which represented by

\[ V(x) = -\Delta \varepsilon(x) \]  

As the dielectric perturbation, \( \Delta \varepsilon(x) \) is the solid state property of the thin film is the main factor that influences the response of the CuS thin film material to electromagnetic wave propagating it, it implies that the absorption coefficient of the propagating wave, \( \psi(x) \) will be dependent on the perturbation since the general fundamental expression of the absorption coefficient of any given thin film for any spectral region of electromagnetic spectrum as it relate photon transmission and absorption is given by

\[ I = I_o e^{-\alpha x} \]

Where \( I \) = intensity of the propagating wave at any instant in the thin film. \( I_o \), the maximum intensity of the wave, \( x \) is the thickness of the thin film.

Using the relation,

\[ \alpha = \frac{2r303(A)}{x} \]  

the band gap is computed based on the solid state properties of the thin film obtained from

\[ \alpha = \sqrt{h \nu - E_g} \]

or

\[ (\alpha h \nu)^2 = A(h \nu - E_g) \]

(Nadeem et al., 2000; Kassim et al., 2010).

With our method, the optical properties such as reflectance, transmittance and absorbance were computed in addition to electrical and optical conductance respectively.

**Result/Discussion**

Fig.1: SEM micrograph of SILAR Deposited CuS Thin film

The micrograph of SILAR and CBD deposited CuS thin film were shown the fig1, and fig.2 respectively. From the observation, as exhibited by the features of the morphology, there is a densely packed film with granular morphology at a particular point. The TEM image taken from the CBD grown CuS thin film revealed appearance of speckled of spherical particles.

Typical X-ray diffraction pattern of CuS thin film is deposited in fig.4 experienced observable peaks at 20°-30° 65°.
The optical characterization of the thin film was carried out using a UV visible spectrophotometer for both SILAR and CBD deposited CuS thin film where it was keenly found that the spectral transmittance is higher within the visible region (600nm) for SILAR deposited film while for CBD deposited thin film, it was seen that the transmittance was higher within the given range, 500nm-650nm with both having very low transmittance in the UV region. The percentage reflectance was discovered to be less than 10% and 15% for both SILAR and CBD deposited CuS thin film respectively. For the computed value, the transmittance...
oscillates within 0.50 and 1.0 for both UV, visible and infrared region of electromagnetic spectrum while the reflectance appeared higher within the UV and decreased within visible region and eventually tends to zero within the infrared region.

The band gap as deduced from the experiment in both cases ranged between 1.25eV to 3.0eV as estimated from the intercept of the linear portion of the plot of $(\alpha h \nu)^2$ against photon energy, $h\nu$ on the photon energy axis. Using the absorption obtained from the computed value which is within 400nm to 450nm, the computed band gap ranged from 2.50eV to 3.0eV. Thus from these observed characteristics as depicted by the thin film especially as regards to its transmittance behavior, it can also be used as solar control characteristics as it can be used to avoid glare as it has low reflectance <10% in the visible region and relatively high reflectance >15% within near infrared region. The observed trend in range of the band gap was base on the variation of the with the thickness of the thin film with other stoichiometrical factors.

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Source of support: Nil; Conflict of interest: None declared